<Interface Science> Solutions and Interfaces

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- Solutions and Interfaces -

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Visitor

Prof BARTHEL, Josef — University of Regensburg, Germany, 16 October 2003

Scope of Research

Structure and dynamics of a variety of ionic and nonionic solutions of physical, chemical, and biological interests are systematically studied by NMR under extreme conditions. High pressures and high temperatures are employed to shed light on microscopic controlling factors for the structure and dynamics of solutions. Vibrational spectroscopic studies are carried out to elucidate structure and orientations of organic and water molecules in ultra-thin films. Static and dynamic NMR of endocrine disruptors, anesthetics, peptides, and proteins in lipid bilayer membranes are also investigated.

Research Activities (Year 2003)

Presentations

Water and Solutions under Extreme Conditions

Noncatalytic Cannizzaro-type Reaction of Acetaldehyde in Supercritical Water, Nagai Y, Wakai C, Matubayasi N, and Nakahara M, International Conference on High Pressure Science and Technology, France, 7-11 July.

A Theoretical Approach to the Solvation Free Energy in the Method of Energy Representation, Matubayasi N, Molecular Liquids: Routes from Local Order to Large-Scale Cooperativity EuroConference, 5 - 10 September.

Multinuclear Magnetic Resonance Spectroscopic Study on Self-diffusion of NaCl and CsCl in Supercritical Water, Nakahara M, International Bunsen Discussion on Dynamics of Molecular Phenomena in Supercritical Fluids, Germany, 1 - 5 September, and 22 related presentations in other meetings and symposia.

Ultra-thin Films

Structure Control of Monolayer Films by Strong Correlations between Single Amide Group and Surface Pressure, Hasegawa T [Nihon University] and Umemura J, Symposium of Grant-in-Aid for Scientific Research for Priority Areas "Dynamic Control of Strongly Correlated Soft Materials", 29 July, and 1 related presentation in other meeting.

NMR of Membrane-Peptide Interactions

High-Resolution NMR Studies on Interactions between Peptides and Phospholipid Bilayers, Kimura T, Okamura E, Matubayasi N, and Nakahara M, Electrochemical Society

Noncatalytic Disproportionation Reaction of Acetaldehyde in Supercritical Water

In supercritical water at 400 °C and 0.5 g/cm^3 (37 MPa), acetaldehyde is found to be transformed without catalysts into ethanol and acetic acid through a disproportionation reaction. The disproportionation competes against the thermal decomposition into methane. Ethanol is generated in excess to acetic acid, and carbon dioxide appears as a product only in the presence of supercritical water. This reaction behavior is explained by considering that carbon monoxide is provided by the acetaldehyde decomposition and leads to the formation of formic acid as a reducing intermediate for acetaldehyde. [Fig. 1]

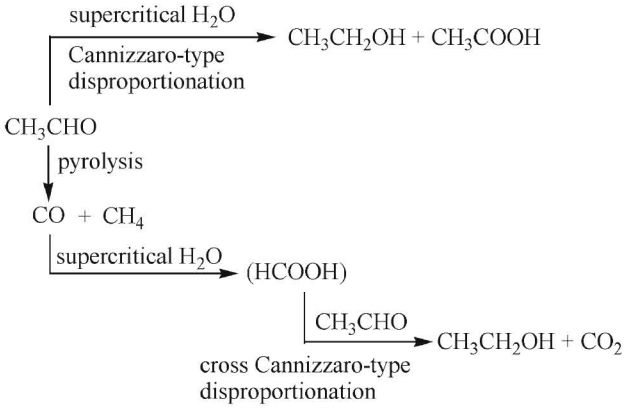

Fig. 1

Binding of a Neuropeptide Achatin-I to Phospholipid Bilayer

Molecular mechanism of the binding of a neuropeptide achatin-I (Gly-D-Phe-Ala-Asp) to large unilamellar vesicles of phosphatidylcholine (PC) is investigated by means of natural-abundance ^{13}C and high-resolution (of 0.01 Hz order) ^1H NMR spectroscopy. The binding equilibrium depends sensitively on the ionization state of the N-terminal $NH3^+$ group in achatin-I. The location of the peptide is the polar region of the PC bilayer interface. [Fig. 2] The side-chain conformational equilibria of the aromatic D-Phe and ionic Asp residues are both affected by the binding; the induced changes are attributed to the peptide-lipid hydrophobic interactions.

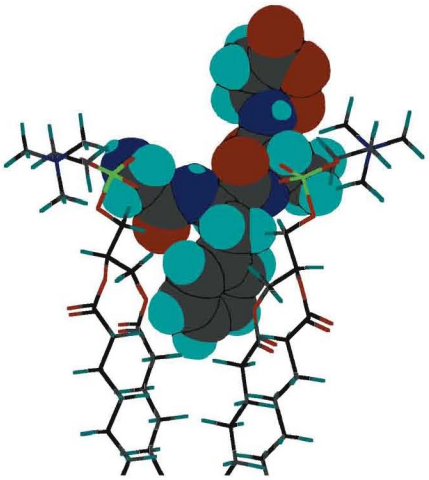

Fig. 2 Molecular picture of the binding of a neuropeptide achatin-I to phospholipid bilayer interface.

Symposium on the Chemistry of Gas-Liquid, Liquid-Liquid, and Liquid-Solid Interfaces, 18 - 19 September, and **5** related presentations in other meetings and symposia.

Grants

Nakahara M, Collaboratory on Electron Correlations - Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2001 - 31 March 2006.

Nakahara M, Development of Multinuclear, High-Temperature, and Diffusion-Measurable NMR Probe and Molecular Analysis of Dynamics of Supercritical Aqueous Solutions, Grant-in-Aid for Creative Scientific Research (A) (2), 1 April 2003 - 31 March 2006.

Nakahara M, "Free-Energy Analysis of Nanoscale Aggregates of Molecules in the Method of Energy Representation", National Research Grid Initiative Project, 1 April 2003 - 31 March 2008.

Matubayasi M, Molecular Studies of Solvation Effect on the Structure and Fluctuation of Biomolecules and their Aggregates, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2003 - 31 March 2008.

Okamura E, Transport of Endocrine Disruptors in Phospholipid Bilayer Membranes, Grant-in-Aid for Scientific Research (C) (2), 1 April 2002 - 31 March 2004.

Wakai C, Inversion of Magnitude Relation of Translational and Rotational Diffusion Coefficients for Organic Acids and Their Ions in Aqueous Solutions, Grant-in-Aid for Scientific Research for Young Scientists (B), 1 April 2002 - 31 March 2004.